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CHIRALITY IN METRIC SPACES

PART 1: An Unifying Symmetry Definition

PART 2: A General Definition of Chirality

- **based on group theory**
- **works in << *NON-EUCLIDEAN* >> Spaces**

Michel Petitjean

CEA/DSV/iBiTec-S/SB2SM (CNRS URA 2096)
F-91191 Gif-sur-Yvette Cedex, France.

Email: petitjean.chiral@gmail.com, michel.petitjean@cea.fr

http://petitjeanmichel.free.fr/itoweb.petitjean.html

http://petitjeanmichel.free.fr/itoweb.petitjean.symmetry.html

PART 1. An Unifying Symmetry Definition

EXAMPLES

Symmetric object: cube, sphere, ...

Symmetric matrix

Symmetric function: $f(x,y) = f(y,x)$
(x,y,f are not necessarily real numbers)

Symmetric function/curve: $f(x) = f(-x)$; $g(x) = - g(-x)$

Symmetric distribution, e.g. Gaussian

Symmetric string or word: AAABBAAA, RADAR, 1234321, ...

Symmetric graph, in the sense of graph theory
(nodes and edges structure, no euclidean coordinates)

<u>In fact, WHAT is indeed symmetric ???</u>

REAL OBJECTS ARE NEVER SYMMETRIC

NO PHYSICALLY EXISTING THING/OBJECT IS SYMMETRIC

ONLY MATHEMATICAL MODELS (in our mind) OF WHAT PHYSICALLY EXISTS CAN BE SYMMETRIC !!

SO, WHAT IS THE MATHEMATICAL MODEL FOR SYMMETRY ?

DO WE NEED SEVERAL MATHEMATICAL MODELS FOR SYMMETRY ?

ONE MAIN MODEL APPLIES TO MOST SITUATIONS

Intuitively, an object is symmetric when it coincides with one of its transforms, but NOT all transforms are allowed:
*** **distances must be preserved** ***

We define a set E.
Its elements may be called points, symbols, digits, letters, etc.

E is NOT a set of objects

An object is a function Y having its input argument in E

Remark 1:
Y has always 1 argument.
E.g. we note Y(x) with x=(x_1, x_2, x_3) rather than Y(x_1, x_2, x_3)

Remark 2:
We don't care about the type of the value returned by Y
(can be a tuple of values of any types, as for x)

We must be able to decide when an object is *identical* to an other object

IDENTITY, EQUALITY, EQUIVALENCE, etc...

The concept above has sense under the following conditions:

(a1) An object is identical to itself.

(a2) IF an object is identical to a second object THEN then this second object is identical to the first one.

(a3) If an object is identical to a second object AND this second object is identical to a third object, THEN the first object is identical to the third object.

The properties (a1), (a2), and (a3) define the so-called *equivalence relation*, inducing the existence of *equivalence classes*.

THE MATHEMATICAL SYMBOL = SATISFIES TO THE THREE PROPERTIES: (a1), (a2), and (a3).

IT WAS CREATED TO HANDLE THE CONCEPT BEHIND THE WORDS: IDENTITY, EQUALITY, EQUIVALENCE, etc...

THE DEBATE ABOUT TERMINOLOGY
(IDENTITY, EQUALITY, EQUIVALENCE)
IS THUS MEANINGLESS.

Basic assumption: **E is a metric space**

It means that we are able to compute the distance between any two elements of E.

Having defined the metric space E and the equality between objects, we need to define the set F of transforms.

Basic assumption about transforms:

Objects defined on E are transformed via transforms over the elements of E

An object Y, which is a function having its input argument x in E, is such that Y(x) is changed to Y(U(x)).

U is to be specified further. For clarity, we will denote U(x) by Ux.

E.g., for a geometric rotational symmetry in the 3D space, the basic assumption about transforms means that the full 3D space is rotated, not the object.

Other assumptions about the transforms

H1: Any element x of E has **at most** one image through a given transform

Should it happen that some x has two images through U,
we would consider that we are in fact dealing with two transforms.

H2: Any element x of E has **at least** one image through a given transform

We consider that any element of E can be transformed by any element of F (F is the set of transforms).
Otherwise there would exist at least one x which could not be transformed by some U in F.
In this situation, we consider that in fact U transforms x into x.

We do not want to privilege the role of an object over the role of its image.

H3: All transforms U of F are injections of E in E

H3 is just H1 applied to U^{-1}

H4: All transforms U of F are surjections of E in E

H4 is just H2 applied to U^{-1}

Collecting H1, H2, H3, H4: U is a bijection from E onto E.

For a finite set E, U is called a permutation.

GROUPS: where ? why ?

Here we consider the operation defined by the composition of bijections

*   The set G of all bijections of E onto E is a group.

E is a metric space:
only distance-preserving bijections (isometries) are retained.

(e.g. reshaping some figure in the Euclidean plane is not convenient in a symmetry study context)

*   The set of all isometries of E onto E is a subgroup of G.

We define F as being this subgroup

The group F acts (operates) on E

An object Y is a function on the metric space E transformed by distance-preserving bijections (isometries) of the elements of E.

Defining Symmetry. 1. More groups

**An object Y is symmetric if there is a bijection U of F,
(with U not equal to the neutral element of F),
such that for any element x of E, Y(Ux)=Y(x)**

We consider the subset S_{YF} of F containing all the elements U of F such that for any element x of E, Y(Ux)=Y(x).

(S_{YF} is not empty because it contains the neutral element of F)

* S_{YF} is shown to be a **subgroup of F**

None of the groups G, F, and S_{YF} are commutative, in general.

Defining Symmetry. 2. More groups (continued)

We can define the transform of an object:

The transform T of an object Y is an object TY
such that for all x in E, $(TY)(x)=Y(U^{-1}x)$

The theory works also with $(TY)(x)=Y(Ux)$

Let Θ be the set of transforms of objects.

The composition of the isometries (elements U of F) induces
the composition of the elements T of Θ.

* Θ is shown to be a **group** acting on the set of objects.

Θ is not commutative, in general.

SYMMETRY OPERATOR:

We define the set S_Y of symmetry operators of Y, as being the subset of Θ containing all elements T such that Y=TY.

Alternate symmetry definition

An object Y is symmetric if the set of its symmetry operators contains at least two elements.

More groups (end).

* S_Y is shown to be a **subgroup** of Θ.

Immediate properties of symmetry operators

For all T in S_Y, T^m=T for any signed integer m.

T_1 and T_2 being two elements of S_Y, they operate commutatively: $T_1T_2Y=T_2T_1Y$.

Moreover the symmetry operators themselves commute:

S_Y is thus a **COMMUTATIVE** group.

So far, we encountered 5 groups during our symmetry study !!!

(G, F, S_{YF}, Θ, S_Y)

All these groups appeared naturally:
no group structure was arbitrarily imposed.

We rediscovered the links between symmetry and group theory.

EXAMPLES

* A real function Y of a real variable x such that Y(x)=Y(-x)
(works even when Y is not a real function)

* A square, a cube, a sphere, etc.: Y takes values in $\{0 ; 1\}$
(Y is the indicator function of the domain)

* Chess board: Y takes values in the set $\{$black, white, nil$\}$

* A real function y of a real variable x such that y(x)=-y(-x)
We have NOT defined the negation operator for functions.
Thus we consider the indicator function Y of the planar curve y(x).

* Probability distribution such as Gaussian, etc.:
We look for the symmetry of the distribution function,
or the symmetry of the density function (if existing).

* Chemistry: e.g., molecular conformer Cl-CHF-Cl.
It can be viewed as a distribution of masses, or a distribution of charges (use a cartesian product), or we can use a set of colors such as $\{$ C, H, F, Cl, nil $\}$. There are other models.

* Palindromas: RADAR, 0001111000, etc.
E is a finite set of symbols. The places of the symbols in a word of length n are numbered 1, 2, ..., n. The distance between the two symbols located respectively at places i and j is $|$j-i$|$.

* Matrices (elements are not necessary numbers): as above, except that places are numbered with two indices i=(i_1,i_2).
Distances are computed with the ususal norm: $\|$j-i$\|$.

* A graph with m nodes (e.g., in chemistry, CH3-CH2-OH):
Y returns the value of the m^2 edges (0/1, colors, weight, etc.).

PART 2. A General Definition of Chirality

Chirality/achirality is usually defined in EUCLIDEAN spaces

An object is achiral is it is identical to one of its image through an *INDIRECT* isometry, i.e. through a composition of any number of translations and of rotations, and of an *ODD* number of mirror inversions.

Question:

Can we extend the classification of euclidean symmetries according to the type (direct/indirect) of isometries they involve, to all non-euclidean symmetries ?

Answer: **YES WE CAN**

It can be defined in any metric space:
no need of the Euclidean structure!

Framework: group theory

<u>GROUP STRUCTURE</u>

Given a group G, we consider the subset of G generated by the products of squared elements of G.

This subset G^+ always exists because it contains at least the neutral element of G.

G^+ is shown to be itself a group and it is called
the ***<u>direct subgroup</u>*** of G.

We define the subset $G^- = G - G^+$

G^- may be void (e.g., when G has only one element).

We assume further that G^- is not empty.

* The product of two elements of G^+ is in G^+

* The product of an element of G^+ by an element of G^- is in G^-

* The product of an element of G^- by an element of G^+ is in G^-

* The product of two elements of G^- is either in G^+ or in G^-

* The involutions of G^- are called ***<u>mirrors</u>***

Thus, the square of a mirror is the neutral element of G, but
the mirror cannot be a product of squared elements of G.

CLASSIFICATION OF ISOMETRIES

The group F of isometries over E can be partitionned into its direct subgroup F^+ and the complement F^- of the direct subgroup to F:
$F^- = F - F^+$

The isometries of F^+ are called ***direct isometries***

The isometries of F^- are called ***indirect isometries***

An object having symmetry due to a direct isometry has ***direct symmetry***

An object having symmetry due to an indirect isometry has ***indirect symmetry***

An object having indirect symmetry is called ***achiral***

An object which is not achiral is called ***chiral***

Extensions:

* When F^- is empty, a symmetric object is called chiral.

* A non symmetric object is called chiral.

<u>EXAMPLES</u>

*   Euclidean spaces:

It is proved that our definition of chirality/achirality is equivalent to the usual one.

*   Strings, words, finite or infinite sequences of symbols:

...ABCABCABC... is symmetric and chiral.

RADAR, ...ABCCBAABCCBA... and ...ABCBAABCBA... are symmetric and achiral.

*   Graphs (nodes and edges):

Graph automorphisms involve permutations.
These latter can be decomposed into independant cycles.

Except the identity,
permutations containing only cycles of length 1 or 2 are mirrors.

A permutation P is in the direct subgroup of isometries
if and only if all its cycles have an odd length.

E.g., the molecular graph of water H-O-H is symmetric and achiral (as the word RADAR), and all molecular graphs containing either methylene groups -CH2- or methyl groups CH3- are symmetric and achiral.

<u>*The symmetries of the molecular graphs must not be confused with the geometric symmetries of the molecular conformers.*</u>

CONCLUSIONS

*   ABOUT PART 1:

We propose our unifying symmetry definition
to be the official one of the ISA.

It is not proved to encompass all practical symmetry situations.
But do we know "all" situations ?
Symmetrists are welcome to provide counterexamples.

A mathematical definition is intended to decide in which situations there is symmetry.
This is a terminology problem, not a math problem.

*   ABOUT PART 2:

We should look at the consequences of our chirality/achirality definition in more spaces, such as hyperbolic spaces.

If it appears to be satisfactory, it may be further proposed to be an official definition, too.